Passivation and Secondary Functionalization of Allyl-Terminated Si(111) Surfaces

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Supporting Information

*1. Computational model of surface **1***

2. XPS comparing surfaces 1 and 2 after treatment by Route A

*3. XPS illustrating the relative oxidation of surfaces **1** and **2** after treatment by Route A*

*1. Computational model of surface **1***

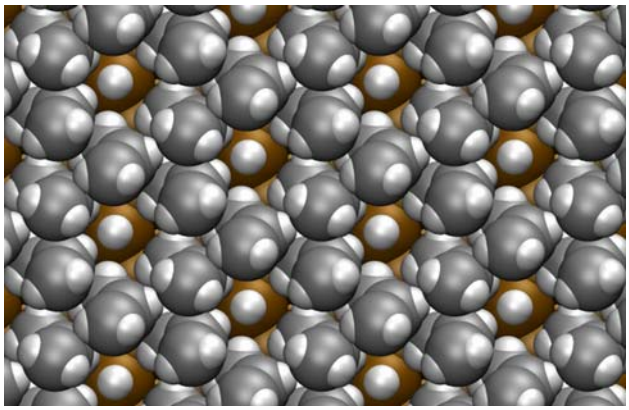

Figure S.1. Energy-minimized molecular mechanics model of surface **1**, indicating the variety of environments which the terminal olefins may inhabit, as well as the space enabling secondary reactions that is provided by the less-than 100% coverage. All atoms are scaled to their van der Waals radii. This calculation was performed in the Cerius^2 program (Accelrys) using the Universal force field and periodic boundary conditions with a 2 x 2 cell.

2. XPS comparing surfaces 1 and 2 after treatment by Route A

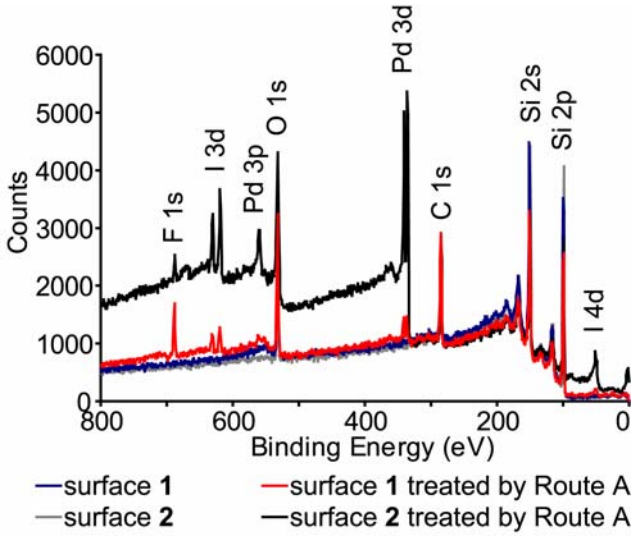

Figure S.2. XPS of surfaces **1** and **2**, before and after treatment by the Heck reaction conditions. Note the increased amount of contamination of surface **2** after treatment, and the smaller F 1s peak, in comparison to surface **1** after treatment.

*3. XPS illustrating the relative oxidation of surfaces **1** and **2** after treatment by Route A*

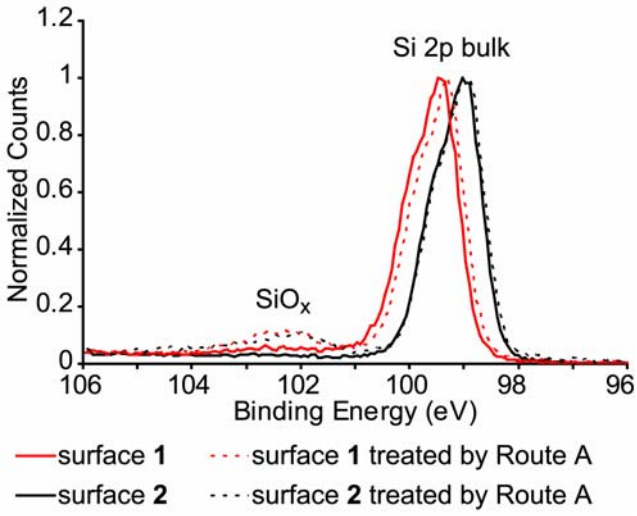

Figure S.3. XPS of the Si 2p region of surfaces **1** and **2** before and after treatment by Route A, the Heck reaction. The SiO_x peak, equivalent to 50% of a monolayer, is noticeable on both surfaces **1** and **2** after treatment in equal amounts. A shift in binding energy is observed between surfaces **1** and **2**.